

# EXAMINATION OF THE ALLOCATIONS OF BUILDING MOLECULES IN THE SINGLE CRYSTAL OF THE PARA-DICHLORBENZOL WITH THE P-DIBROMOBENZENE SOLID SOLUTION BY THE METHOD OF THE RAMAN EFFECT OF LIGHT DEPENDING ON REQUIREMENTS OF SELECTION

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Allocation of molecules of para-dichlorbenzol in equimolar single crystals of para-dichlorbenzol with p-dibromobenzene solid solutions grown by the Bridgmen's method is studied. It is shown, that the mutual concentration of builders longwise an exemplar depends on requirements of selection. Probably as a uniform modification of concentration of builders along an exemplar, and a wavy modification of concentration. Critical speed at a modification of character of allocation made  $15.0 \cdot 10^{-6}$  cm/s at a lapse rate of temperature  $dT/dl=7.7$  grad/cm.

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In a number of publications [1] it is shown, that for two-component solid solutions depending on requirements of selection of single crystals on method Bridgmen it is possible both a uniform modification of concentration of builders, and wavy. In operation it speaks periodic appearance and wedging out of blocks during propagation boundaries which segregation of impurity takes place. These examinations were spent on junction  $^{14}\text{H}_{14}$  and  $\text{C}_{14}\text{H}_{10}$ . Operation by [2] us it is carried out examination of solid solutions of para-dichlorbenzol with a p-dibromobenzene grown on method Bridgmen at velocities of pulling down of dish  $V=8.3 \cdot 10^{-6}$ – $8.9 \cdot 10^{-6}$  cm/s and a lapse rate temperature  $dT/dl=7.6$ – $7.7$  grad/cm. Monotone allocation of impurity has been discovered. Therefore in the yielded operation are carried out examinations for various velocities of pulling down of dish. To define nonmonotone allocation of impurity in studied mix-crystals takes place at a modification of requirements of selection.

It promotes understanding of the mechanism of crystal growth and will enable to influence it.

P-dibromobenzene and para-dichlorbenzol ( $\alpha$ -modification), crystallizes in centrosymmetric space group  $P2_1/a$  with two molecules in a low level cell. These chips were researched by a X-ray diffraction method [3], methods of a Raman effect of light [4] and a nuclear quadrupole resonance [5]. X-ray diffraction data on the mix-crystals studied in operation, us it is not revealed. These mix-crystals have been selected because their components are isomorphic among themselves and form solid solutions at any concentrations of builders. Single crystals of solid solutions have been grown on method Bridgmen.

In the yielded operation the method of a Raman effect of light which allows to judge on spectrums of the lattice and intramolecular oscillations character of layout of molecules of impurity among molecules of the main chip is used.

In Fig. 1 spectrum of the lattice oscillations the mixed

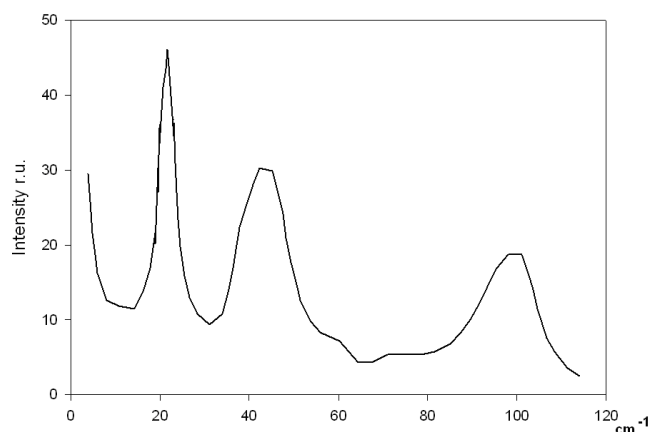


FIG. 1: Spectrum of the lattice oscillations.

chip of a p-dibromobenzene with para-dichlorbenzol is reduced at concentration 50 pier. % of builders. The spectrum of mix-crystals is similar to spectrums of builders that speaks about allocation of impurity as substitution.

The value of concentration of impurity in the grown single crystals of solid solutions was defined on relative intensity of the valence intramolecular oscillations. According to operation [6] line in spectrum of a p-dibromobenzene with frequency of  $\nu = 212.0 \text{ cm}^{-1}$  corresponds to valence vibration C-Br, and a line with frequency of  $\nu = 327.0 \text{ cm}^{-1}$  in para-dichlorbenzol – to valence vibration C-Cl.

In Fig. 2 spectrums of intramolecular oscillations (in the field of from 150 up to  $400 \text{ cm}^{-1}$ ) a p-dibromobenzene (1), para-dichlorbenzol (2) and studied mix-crystals are presented at equimolecular concentrations of para-dichlorbenzol in a p-dibromobenzene (3). Using a relation intensity the symmetric valence vibrations in mix-crystals, the modification of concentration of builders longwise single crystals is revealed. Examinations of different exemplars it was spent at the same parameters of a

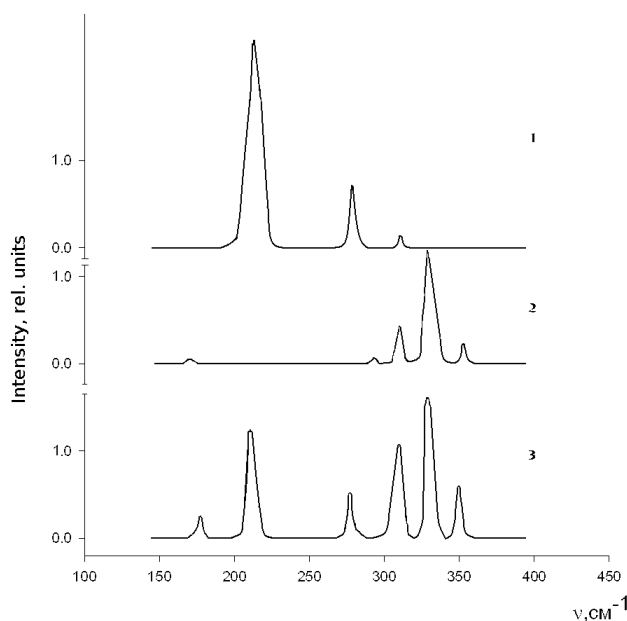


FIG. 2: Spectrum of intramolecular oscillations.

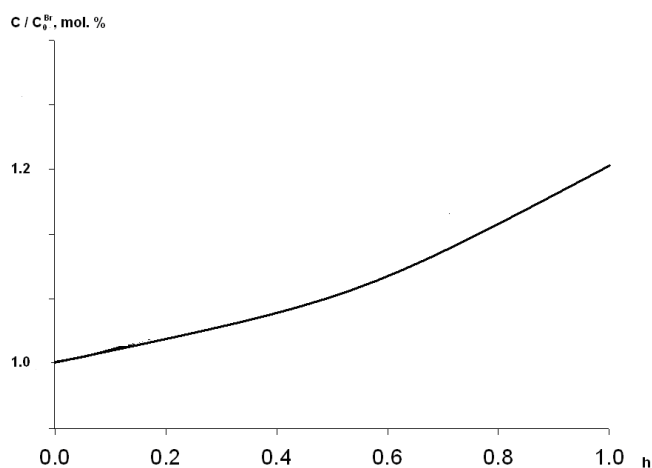


FIG. 3: Allocation of impurity of para-dichlorbenzol and p-BromoChlorobenzene longwise (h) the mixed chip at low speed of propagation.

data-acquisition equipment. In operation concentration of builders was measured in molar unities.

The single crystal was grown in a glass tube in diameter  $d = 1$  cm and length  $h = 10$  cm with the plucked capillary. In a handset put mother substances in the necessary percentage. After that from a handset pumped out air, and she was sealed off.

The handset with substance was omitted in the crystallizing furnace with velocity  $V = 8.3 \cdot 10^{-6} - 8.9 \cdot 10^{-6}$  cm/s. The lapse rate of temperature of the furnace was set by

various winding of a heating coil and made  $dT/dl = 7.6 - 7.7$  a grad/cm.

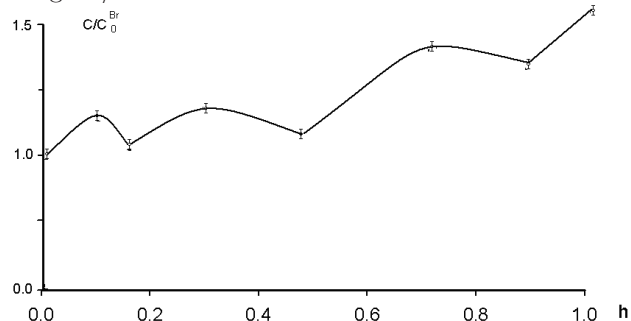


FIG. 4: Allocation of impurity of para-dichlorbenzol and p-BromoChlorobenzene longwise (h) the mixed chip at a high speed of propagation.

In Fig. 3 association of relative concentration of a p-dibromobenzene to para-dichlorbenzol is shown. The initial concentration of p-dibromobenzene  $C_0^{Br}$  in fusion mixture of the researched exemplars made 50 pier. %. Apparently, in process of propagation of single crystals concentration of impurity increases.

In Fig. 4 graphics of allocation of a builder of para-dichlorbenzol  $C/C_0^{Br}$  on an axis of a single crystal in solid solutions are presented at greater growth rate  $V = 20.0 \cdot 10^{-6}$  cm/s and a lapse rate of temperature  $dT/dl = 7.7$  grad/cm.

As we see Allocation of builders has wavy character. The velocity of pulling down of dish at which is broken monotone allocation makes in our case  $V 15.0 \cdot 10^{-6}$  cm/s.

So, changing requirements of selection it is possible to change allocation of molecules of impurity thus probably as a uniform modification of concentration of all builders along an exemplar, and a wavy modification of concentration of two substances that will affect long-distance and short-range order of layout of molecules.

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